5-octyl-dihydrofuran-2(3H)-thione

Inchi: InChI=1S/C12H20OS/c1-2-3-4-5-6-7-8-11-9-10-12(14)13-11/h9H,2-8,10H2,1H3
InchiKey: FNNJWMAXWIIUGC-UHFFFAOYSA-N
Formula: C12H20OS
SMILES: CCCCCCCCC1=CCC(=S)O1
Mol. weight [g/mol]: 212.35

Physical Properties

Property code	Value	Unit	Source
gf	119.48	kJ/mol	Joback Method
hf	-180.78	kJ/mol	Joback Method
hfus	34.55	kJ/mol	Joback Method
hvap	55.81	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.369		Crippen Method
mcvol	182.700	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	1810.00		NIST Webbook
ripol	2593.00		NIST Webbook
tb	597.64	K	Joback Method
tc	801.99	K	Joback Method
tf	343.66	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.31	J/mol×K	597.64	Joback Method
cpg	469.77	J/mol×K	631.70	Joback Method
cpg	484.36	J/mol×K	665.76	Joback Method
cpg	498.11	J/mol×K	699.81	Joback Method
cpg	511.09	J/mol×K	733.87	Joback Method
cpg	523.35	J/mol×K	767.93	Joback Method
cpg	534.95	J/mol×K	801.99	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R422525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume